* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

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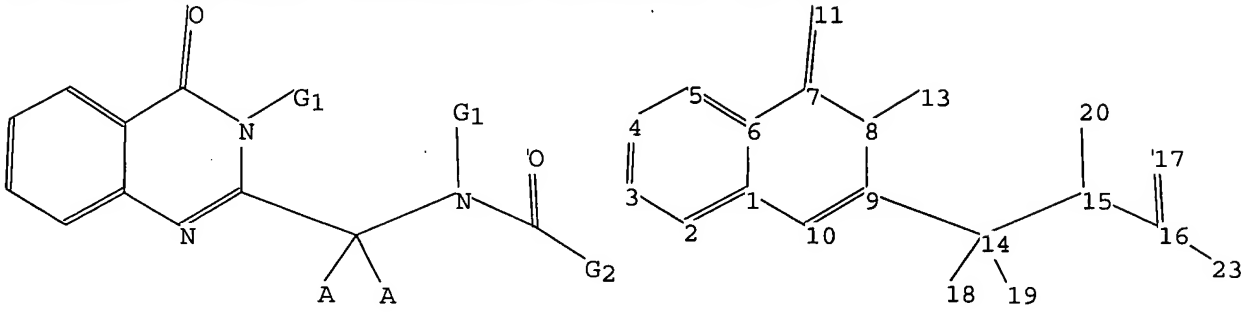

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ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
7-11 8-13 9-14 14-15 14-18 14-19 15-16 15-20 16-17 16-23
ring bonds :
1-2 1-6 1-10 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10
exact/norm bonds :
1-10 6-7 7-8 7-11 8-9 8-13 9-10 14-15 14-18 14-19 15-16 15-20 16-17
16-23
exact bonds :
9-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

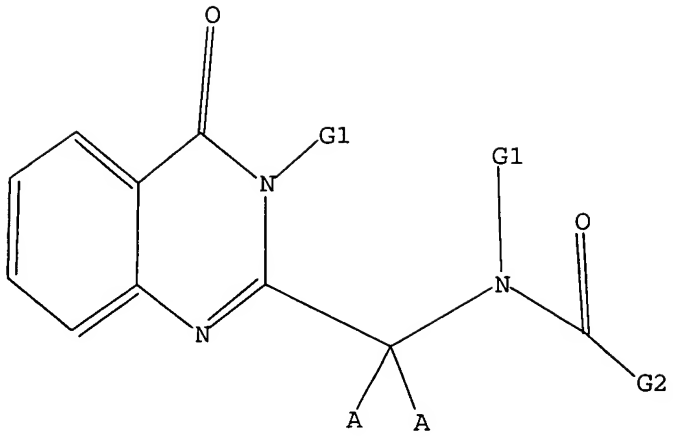
G1:H,Cy,Ak

G2:H,O,N,Cy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 23:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 H,Cy,Ak

G2 H,O,N,Cy,Ak

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 full
L3             1 SEA SSS FUL L1

=> file ca


=> s l3
L4             1 L3

=> d ibib abs hitstr
```

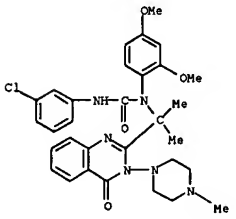
L4 ANSWER 1 OF 1 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 141:325172 CA
TITLE: Quinazolinone-based fungal efflux pump inhibitors. Part 1: Discovery of an (N-methylpiperazine)-containing derivative with activity in clinically relevant Candida spp.
AUTHOR(S): Lemoine, Remy C.; Glinka, Tomasz W.; Watkins, William J.; Cho, Aesop; Yang, Jessie; Iqbal, Nadeem; Singh, Rajeshwar; Madsen, Deidre; Lolans, Karen; Lomovskaya, Olga; Oza, Uma; Dudley, Michael N.
CORPORATE SOURCE: Essential Therapeutics, Inc., Mountain View, CA, 94043, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(20), 5127-5131
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The discovery of a series of quinazolinone-based fungal efflux pump inhibitors by high-throughput screening for potentiation of fluconazole in C. albicans is described. Attempts to improve the aqueous solubility of screening hits led to the discovery of an analog with greatly improved phys. properties and activity against clin.-relevant Candida spp.

IT 770743-58-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(N-methylpiperazine-containing quinazolinone derivative, efflux pump inhibitors in clin. relevant Candida spp.)

RN 770743-58-3 CA
CN Urea, N'-(3-chlorophenyl)-N-[1-[3,4-dihydro-3-(4-methyl-1-piperazinyl)-4-oxo-2-quinazolinyl]-1-methylethyl]-N-(2,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 1 OF 1 CA COPYRIGHT 2005 ACS on STN (Continued)

10/773,602

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=> s l1 full
FULL SEARCH INITIATED 09:26:43 FILE 'CASREACT'
SCREENING COMPLETE - 957 REACTIONS TO VERIFY FROM 59 DOCUMENTS

100.0% DONE 957 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L1 (0 REACTIONS)

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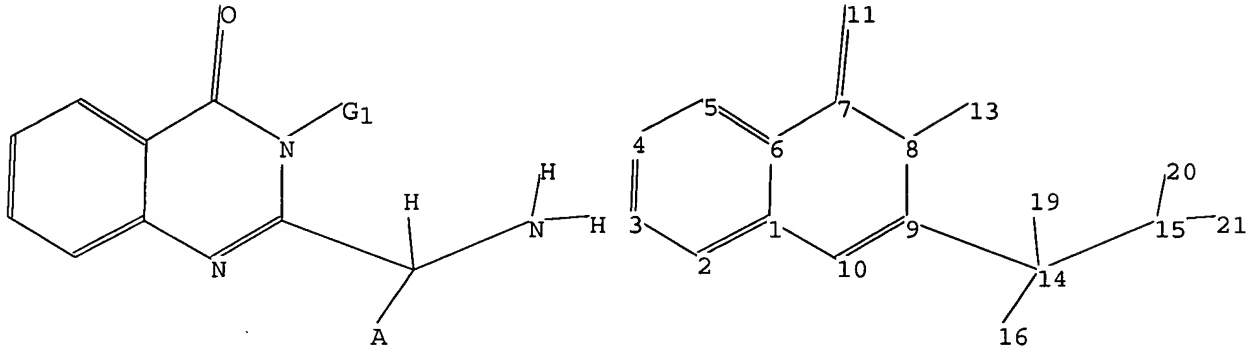

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ring nodes :
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chain bonds :
7-11 8-13 9-14 14-15 14-16 14-19 15-20 15-21
ring bonds :
1-2 1-6 1-10 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-10
exact/norm bonds :
1-10 6-7 7-8 7-11 8-9 8-13 9-10 14-15 14-16
exact bonds :
9-14 14-19 15-20 15-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,Cy,Ak

G2:H,O,N,Cy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS

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L7      STRUCTURE UPLOADED

=> file reg

=> s l7 full
L9            23 SEA SSS FUL L7

=> file ca


=> s l9
L10           19 L9

=> d ibib abs fhitstr 1-19
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L10 ANSWER 1 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 141:89125 CA
TITLE: Preparation of oxodiazepanylquinazolinones as modulators of KSP kinesin activity for treatment of proliferative disease.
INVENTOR(S): Bergnes, Gustave; Dhanak, Dashyant; Knight, Steven David; Lu, Pu Ping; Morgans, David J., Jr.; Newlander, Kenneth Allen
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; Cytokinetics
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004055008	A1	20040701	WO 2003-US39708	20031212
W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, EG, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, OM, PH, PL, RO, SC, SG, TN, TT, UA, US, UZ, VN, YU, ZA				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2002-433494P P 20021213
US 2002-435001P P 20021219
OTHER SOURCE(S): MARPAT 141:89125
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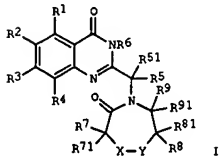
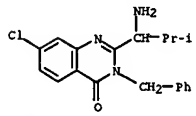


I

AB Title compds. [I; R1-R4 = H, halo, OH, NO2, cyano, (substituted) alkyl, alkoxy, aryl, heteroaryl, etc.; R5, R51 = H, (substituted) alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl; R5R51C = 3-7 membered carbocyclyl; R6 = H, (substituted) alkyl, aryl, aralkylo, heteroaryl, heteroaralkyl; R7, R71, R8, R81, R9, R91 = H, (substituted) alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl; X, Y = CR10R11, NR12, O, S; R10, R11 = H, (substituted) alkyl, aryl, heteroaryl; R12 = H, (substituted) alkyl, aralkyl, heteroaralkyl, alkylcarbonyl, arylcarbonyl, heteroarylcarbonyl,

L10 ANSWER 1 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)
aralkylcarbonyl, heteroaralkylcarbonyl, alkoxycarbonyl, etc.], were prepd. Thus, N-(2-aminoethyl)-N-[1-(3-benzyl-7-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]acrylamide (prepn. given) was refluxed overnight in MeOH to give 3-benzyl-7-chloro-2-[2-methyl-1-(7-oxo-1,4-diazepan-1-yl)propyl]-3H-quinazolin-4-one. Some I inhibited cell proliferation with GI50 <10 nM.
IT 336119-88-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of oxodiazepanylquinazolinones as modulators of KSP kinesin activity)
RN 336119-88-1 CA
CN 4(3H)-Quinazolinone, 2-(1-amino-2-methylpropyl)-7-chloro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 141:23488 CA
TITLE: A preparation of pyrazino[2,1-b]quinazolone derivatives useful as multidrug resistance modulators
AUTHOR(S): Kokosi, Jozsef; Almasi, Janos; Pokanyi, Benjamin; Hermecz, Istvan
CORPORATE SOURCE: Gyogyszereszi Kemiai Intezet, Semmelweis Egyetem, Budapest, Russia
SOURCE: Acta Pharmaceutica Hungarica (2003), 73(1), 29-39
CODEN: APHGAO; ISSN: 0001-6659
PUBLISHER: Magyar Gyogyszereszeti Tarsasag
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
OTHER SOURCE(S): CASREACT 141:23488
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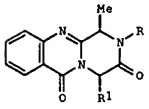

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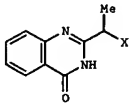
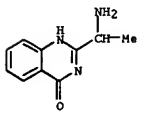


II

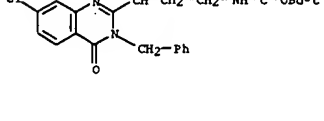
AB An exploration for new MDR-modulators utilizing pyrazino[2,1-b]quinazolones as scaffolds disclosed after systematic synthetic investigation highly hydrophobic N-substituted derivs. as readily accessible active tricyclic compds. (no biol. data). A versatile synthesis of 2-substituted-1,2,3,4-tetrahydro-6H-pyrazino[2,1-b]quinazoline-3,6-diones is presented starting from 2,3-substituted quinazolones. The new compds. have been characterized by elemental analyses, NMR, and in some cases by 13C ruler, and X-ray investigations. For instance, pyrazino[2,1-b]quinazoline derivative I was prepared via amination of quinazoline II (X = Br) by RNH2, N-acetylation of the obtained amine II (X = NHR) by YCH(R1)C(O)Y (R1 is H or Me; Y is Cl or Br), and subsequent heterocyclization of the obtained amide II [X = N(R)C(O)C(Y)R1].
IT 172420-42-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of pyrazino[2,1-b]quinazolone derivs. useful as multidrug resistance modulators)
RN 172420-42-7 CA
CN 4(1H)-Quinazolinone, 2-(1-aminoethyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 3 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 140:139471 CA
TITLE: Preparation of of quinazolinone-like derivatives to treat cellular proliferative diseases
INVENTOR(S): Bergnes, Gustave; Smith, Whitney W.; Yao, Bing; Morgans, David J., Jr.; MacDonald, Andrew
PATENT ASSIGNEE(S): Cytokinetics, Inc., USA
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009036	A2	20040129	WO 2003-US23319	20030723
WO 2004009036	A3	20040819		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20041429 49	A1	20040722	US 2003-626012	20030723

PRIORITY APPLN. INFO.: US 2002-398224P P 20020723
OTHER SOURCE(S): MARPAT 140:139471
AB The invention relates to quinazolinone-like derivs. that are inhibitors of the mitotic kinesin KSP and are useful in the treatment of cellular proliferative diseases, for example cancer, hyperplasias, restenosis, cardiac hypertrophy, immune disorders and inflammation. Preparation of 3-Benzyl-7-chloro-2-(3-benzyl-2-oxohexahydropyrimidin-4-yl)-3H-quinazolin-4-one is included.
IT 651323-46-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinazolinone derivs. to treat cellular proliferative diseases)
RN 651323-46-5 CA
CN Carbamic acid, [3-amino-3-[7-chloro-3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 4 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 140:5063 CA
TITLE: 2-[1-(Imidazol-1-yl)alkyl]-3H-quinazolin-4-one derivatives, pharmaceutical compositions containing them, and methods of their use as KSP kinesin inhibitors for the treatment of cellular proliferative diseases
INVENTOR(S): Feng, Bainian; Bergnes, Gustave; Morgans, David J. C., Jr.; Dhanak, Dashyant; Knight, Steven David; Darcy, Michael Gerard
PATENT ASSIGNEE(S): Cytokinetics, Inc., USA; Smithkline Beecham Corporation
SOURCE: PCT Int. Appl., 97 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003097053	A1	20031127	WO 2003-US14787	20030508
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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US 2004077668	A1	20040422	US 2003-435069	20030508
PRIORITY APPLN. INFO.:			US 2002-379531P	P 20020509
OTHER SOURCE(S):	MARPAT 140:5063			

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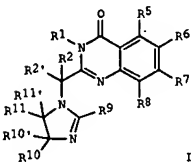
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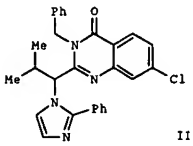

II

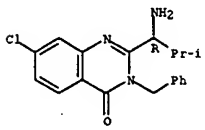
AB Compds. useful for treating cellular proliferative diseases and disorders by modulating the activity of KSP (kinesin-like spindle protein), and especially

L10 ANSWER 4 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)
human KSP, are disclosed (no data). In particular, compds. I are claimed [wherein: R1 = H, (un)substituted alkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl; R2, R2' = H, (un)substituted alkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl; or R2R2' = (un)substituted 3- to 7-membered ring; R5, R6, R7, R8 = H, (un)substituted alkyl or alkoxy, halo, OH, NO2, cyano, dialkylamino, alkylsulfonyl, alkylsulfonamido, alkylthio, carboxyalkyl, carboxamido, aminocarbonyl, (un)substituted aryl, aryloxy, heteroaryl, or heteroaryloxy; R9 = H, (un)substituted alkyl, aryl, aralkyl, or heteroaryl; R10, R10', R11, R11' = H, (un)substituted alkyl, aryl, or aralkyl; or R10'R11' = pi bond; including single and mixed stereoisomers and pharmaceutically acceptable salts and/or solvates]. Approx. 60 compds. I are described in examples. Compds. I having (R)-configuration at the stereogenic center bearing R2 are preferred for reasons of greater potency than the (S)-isomers. For instance, 2-(1-amino-2-methylpropyl)-3-benzyl-7-chloro-3H-quinazolin-4-one underwent a sequence of N-alkylation at amino with BrCH2CH(OMe)2 and K2CO3 (59%), amidation of the resultant secondary amine with PhCOCl and Et3N (54%), and deprotection/cyclocondensation with NH4OAc in refluxing AcOH (23%) to give invention compd. II. Compds. I are said to be active against human ovarian cancer cells SKOV3 in vitro. Visual inspection revealed that the compds. caused cell cycle arrest in the prometaphase stage of mitosis; DNA was condensed and spindle formation had initiated, but arrested cells uniformly displayed monopolar spindles, indicating that there was an inhibition of spindle pole body sepn.

IT 336113-57-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of (imidazolylalkyl)quinazolinone derivs. as KSP kinesin inhibitors for the treatment of cellular proliferative diseases)

RN 336113-57-6 CA
CN 4(3H)-Quinazolinone, 2-[(1R)-1-amino-2-methylpropyl]-7-chloro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 139:261313 CA
TITLE: Quinazolinone amide compounds as modulators of nuclear receptors, particularly farnesoid X receptor (FXR) and/or orphan nuclear receptors, and their preparation, pharmaceutical compositions, and methods of use
INVENTOR(S): Martin, Richard; Kahl, Jeffery Dean; Flatt, Brenton Todd; Griffith, Ronald
PATENT ASSIGNEE(S): X-Ceptor Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 204 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003076418	A1	20030918	WO 2003-US6793	20030304
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EP 1521746	A1	20050413	EP 2003-726031	20030304
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PRIORITY APPLN. INFO.:			US 2002-363132P	P 20020307
			WO 2003-US6793	W 20030304
OTHER SOURCE(S):	MARPAT 139:261313			

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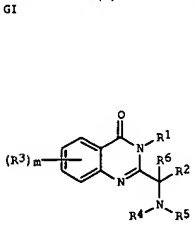
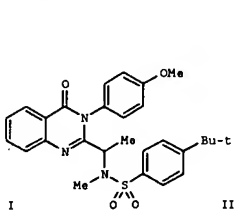

I

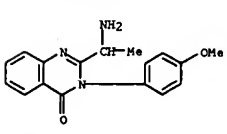

II

AB Compds., pharmaceutical compns., and methods for modulating the activity of nuclear receptors are provided. In particular, amide-containing quinazolinones are provided for modulating the activity of farnesoid X receptor (FXR) and/or orphan nuclear receptors. The disclosed compds. include I [m = 0-4; R1 = H, (un)substituted alk(en/yn)yl, (hetero)aryl, cycloalkyl(alkyl), (hetero)aralkyl, heterocyclyl(alkyl) (preceding groups designated as group A), OH or derivs., NH2 or derivs.; R2, R6 =

L10 ANSWER 5 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)
(independently) group A, or R2R6 = (un)substituted alkylene; R4, R5 = (independently) group A, OH or derivs, NH2 or derivs., various acyl, sulfinyl, sulfonyl, or phosphoryl groups, etc.; or R4R5 (un)substituted alkylene, alkenylene, alkenylene(oxy/aza)alkenylene; or any of R2R5, R2R4, R5R6, or R4R6 form 4- to 7-membered, (un)substituted heteroaryl or heterocyclyl group; R3 = (independently) halo, pseudohalo, group A, NH2 or derivs., OH or derivs., SH or derivs., various acyl, thioacyl, imidoyl, sulfinyl, or sulfonyl groups; or adjacent R3R3 = (un)substituted alkylene, alkenylene, alkylenedioxy, thioalkylenoxy, alkylenedithioxy; including stereoisomers, racemates, mixts., and pharmaceutically acceptable derivs.; with one exception compd.]. Over 300 specific compds. were prepd. and claimed by name. Ten of the most preferred compds. are named. The compds. are useful for treating diseases and disorders selected from: hypercholesterolemia, hyperlipoproteinemia, hypertriglyceridemia, lipodystrophy, hyperglycemia, diabetes mellitus, dyslipidemia, atherosclerosis, gallstone disease, acne vulgaris, acneiform skin conditions, diabetes, Parkinson's disease, cancer, Alzheimer's disease, inflammation, immunol. disorders, lipid disorders, obesity, conditions characterized by a perturbed epidermal barrier function, hyperlipidemia, cholestasis, peripheral occlusive disease, ischemic stroke, obesity, disease states assocd. with elevated cholesterol levels, conditions of disturbed differentiation or excess proliferation of the epidermis or mucous membrane, and cardiovascular disorders. For instance, Me anthranilate was N-amidated with 2-chloropropionyl chloride (97%), followed by sapon. of the ester (97%), and amidation/cyclocondensation of the resultant acid using p-anisidine and PCl3 (72%), to give 2-(1-chloroethyl)-3-(4-methoxyphenyl)-3H-quinazolin-4-one. This intermediate chloride was aminated with methylamine in THF (99%), and the obtained secondary amine was sulfonylated with 4-tert-butylbenzenesulfonyl chloride and TEA in DCM (92%), to give preferred invention compd. II. In an FRET assay for binding to human FXR (ligand-binding domain, fused to glutathione-S-transferase), II had an EC50 of about 300 nM. In an FXR/ECREx7 co-transfection assay using African green monkey kidney cells, II had an efficacy of 190% relative to high control (chenodeoxycholic acid).

IT 602318-88-7P, 3-(4-Methoxyphenyl)-2-methylaminomethyl-3H-quinazolin-4-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate and drug candidate; preparation of quinazolinone amides as farnesoid X and/or orphan nuclear receptor modulators)

RN 602318-88-7 CA
CN 4(3H)-Quinazolinone, 2-(1-aminoethyl)-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 19 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 139:214481 CA
TITLE: Syntheses of enantiomerically pure quinazolinones
INVENTOR(S): Bergnes, Gustav; Ha, Edward; Yiannikourous, George; Kalaritis, Panos; Yonce, Brandon E.; Welday, Kurt Alan, Jr.
PATENT ASSIGNEE(S): Cytokinetics, Inc., USA; SmithKline Beecham Corp.
SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003070701	A2	20030828	WO 2003-US4713	20030214
WO 2003070701	A3	20031016		
WO 2003070701	B1	20031218		

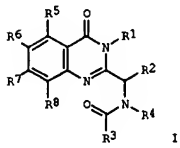
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2475879	AA	20030828	CA 2003-2475879	20030214
US 2004067969	A1	20040408	US 2003-366828	20030214
EP 1480980	A2	20041201	EP 2003-709135	20030214

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.:	US 2002-357244P	P 20020215
	US 2002-380746P	P 20020514
	WO 2003-US4713	W 20030214

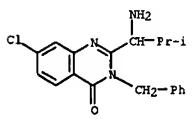
OTHER SOURCE(S): MARPAT 139:214481
GI



I

AB The present invention provides intermediates, synthetic methods and novel

L10 ANSWER 6 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)



L10 ANSWER 6 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)

quinazolinone (shown as I; e.g. (R)-N-(3-aminopropyl)-N-[1-(3-benzyl-7-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]-4-methylbenzamide) compns. of matter, which are inhibitors of the mitotic kinesin KSP (no data) and are useful in the treatment of cellular proliferative diseases, for example cancer, hyperplasias, restenosis, cardiac hypertrophy, immune disorders and inflammation (no data); only the compds., compns. of matter and synthetic methods are claimed. The method comprises contacting HO2CCH(R2)NHX (R2 = oxaalkyl or (un)substituted alkyl, aryl, alkylaryl, heteroaryl, or alkylheteroaryl; X = H, protecting group (e.g. Boc, CBZ, phthalide, allyloxycarbonyl, 2,2,2-trichloroethoxycarbonyl); e.g. valine) with iso-Bu chloroformate followed by contacting the resulting product with (un)substituted 2-aminobenzoic acids to give I. Eight example prepns. of I are included. For example, (S)-[1-(3-benzyl-7-chloro-4-oxo-3,4-dihydroquinazolin-2-yl)-2-methylpropyl]carbamic acid tert-Bu ester was prepd. starting from N-Boc-L-valine and involving intermediates 2-[[2-[(tert-butoxycarbonyl)amino]-L-3-methylbutyryl]amino]-4-chlorobenzoic acid, (S)-[1-(7-chloro-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)-2-methylpropyl]carbamic acid tert-Bu ester, (S)-[1-[[(2-benzylcarbamoyl-5-chlorophenyl)imino]methyl]-2-methylpropyl]carbamic acid tert-Bu ester (in mixt. with the final product). In the key step, to 2-[[2-[(tert-butoxycarbonyl)amino]-L-3-methylbutyryl]amino]-4-chlorobenzoic acid was added 13.2 mL (0.1 mol) of iso-Bu chloroformate over 15 min (internal temp. 5°) followed by the addn. of 11.1 mL (0.1 mol) of anhyd. N-methylmorpholine over 15 min at 0°; the mixt. was stirred for an addnl. hour at 0° to give (S)-[1-(7-chloro-4-oxo-4H-benzo[d][1,3]oxazin-2-yl)-2-methylpropyl]carbamic acid tert-Bu ester. For I: R1 is H or (un)substituted alkyl, aryl, alkylaryl, heteroaryl, or alkylheteroaryl; R3 is H, oxaalkyl, R9O-, R9NH- or (un)substituted alkyl, aryl, alkylaryl, heteroaryl, alkylheteroaryl, or oxaalkylaryl; R4 is H or (un)substituted alkyl, aryl, alkylaryl, heteroaryl, or alkylheteroaryl; R5, R6, R7 and R8 = H, hydroxy, (un)substituted alkyl, alkoxy, halogen, fluoroalkyl, nitro, cyano, amino, alkylamino, dialkylamino, alkylsulfonyl, alkylsulfonamido, sulfonamidoalkyl, sulfonamidoaryl, alkylthio, carboxyalkyl, carboxamido, aminocarbonyl, aryl or heteroaryl; and R9 is (un)substituted alkyl, aryl, alkylaryl, heteroaryl, or alkylheteroaryl. The compns. of matter comprise I and detectable amts. of ≥1 unreacted starting materials and/or a cyclo-dehydration reagent; they are claimed, presumably because it is important to monitor the purity of pharmaceutical compds. for the presence of such materials, which presence comprises a way of detecting use of a process of the invention.

IT **336119-88-1P**, 2-(1-Amino-2-methylpropyl)-3-benzyl-7-chloro-3H-quinazolin-4-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(resolution; syntheses of enantiomerically pure quinazolinones)

RN 336119-88-1 CA
CN 4(3H)-Quinazolinone, 2-(1-amino-2-methylpropyl)-7-chloro-3-(phenylmethyl)-(9CI) (CA INDEX NAME)

L10 ANSWER 7 OF 19 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 137:337912 CA
TITLE: Preparation of purinylquinazolinones as inhibitors of human phosphatidylinositol 3-kinase delta
INVENTOR(S): Sadhu, Chanchal; Dick, Ken; Treiberg, Jennifer; Sowell, C. Gregory; Kesicki, Edward A.; Oliver, Amy
PATENT ASSIGNEE(S): ICOS Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 86 pp., Cont.-in-part of U.S. Ser. No. 841,341.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002161014	A1	20021031	US 2001-27591	20011019
US 6667300	B2	20031223		
US 6518277	B1	20030211	US 2001-841341	20010424
WO 2003035075	A1	20030501	WO 2002-US27240	20020827

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

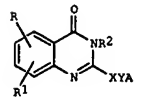
EP 1438052	A1	20040721	EP 2002-757407	20020827

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK

JP 2005509635	T2	20050414	JP 2003-537642	20020827
ZA 2002008698	A	20031010	ZA 2002-8698	20021028
US 2003195211	A1	20031016	US 2003-337192	20030106
US 6800620	B2	20041005		
US 2004266780	A1	20041230	US 2003-697912	20031030

PRIORITY APPLN. INFO.:	US 2000-199655P	P	20000425
	US 2000-238057P	P	20001005
	US 2001-841341	A2	20010424
	US 2001-27591	A	20011019
	WO 2002-US27240	W	20020827

OTHER SOURCE(S): MARPAT 137:337912
GI



I

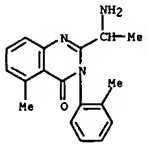
AB A method of disrupting leukocyte function comprises administration of

L10 ANSWER 7 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)
title compds. [I; X = C(Rb)2, CH2CHRb, CH:CRb; Rb = H, alkyl, heteroalkyl, aryl, heteroaryl, aralkyl, etc.; Y = null, S, SO, SO2, NH, O, CO, CO2, NHCOCH2S; R, R1 = H, alkyl, aryl, heteroaryl, halo, etc.; RR1 = atoms to form a 3-4 membered alkylene, alkenylene chain; R2 = H, (substituted) alkyl, cycloalkyl, heterocycloalkyl, alkylenecycloalkyl, alkenyl, alkylenearyl, aryl, heteroaryl, etc.; A = (substituted) mono- or bicyclic ring system contg. ≥2 N atoms and in which ≥1 ring is arom.]. Thus, dose-dependent decrease in histamine release from basophils when stimulated with anti-IgE was 100% at 1,000 nM, with an EC50 of about 25 nM for I (Y = S, R = 5-Me, R1 = H, R2 = 2-ClC6H4, R3 = H; S connected to 6-position of purine ring; prepn. given).

IT 371244-09-6P, 4(3H)-Quinazolinone, 2-(1-aminoethyl)-5-methyl-3-(2-methylphenyl)-
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of purinylquinazolinones as inhibitors of human phosphatidylinositol 3-kinase delta)

RN 371244-09-6 CA

CN 4(3H)-Quinazolinone, 2-(1-aminoethyl)-5-methyl-3-(2-methylphenyl)- (9CI) (CA INDEX NAME)



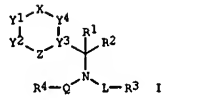
L10 ANSWER 8 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 137:337907 CA
TITLE: Preparation of N-(heteroarylalkyl)acylamides as CXCR3 antagonists for treatment of inflammatory or immune conditions
INVENTOR(S): Medina, Julio C.; Johnson, Michael G.; Li, An-Rong; Liu, Jiwen; Huang, Alan Xi; Zhu, Liusheng; Marcus, Andrew P.
PATENT ASSIGNEE(S): Tularik Inc., USA
SOURCE: PCT Int. Appl., 205 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002083143	A1	20021024	WO 2001-US47850	20011211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2431553	AA	20021024	CA 2001-2431553	20011211
US 2002169159	A1	20021114	US 2001-15532	20011211
EP 1343505	A1	20030917	EP 2001-273533	20011211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004536796	T2	20041209	JP 2002-580947	20011211
US 2003069234	A1	20030410	US 2002-164690	20020606
US 6794379	B2	20040921		
US 2003055054	A1	20030320	US 2002-231895	20020829
NO 2003002612	A	20030805	NO 2003-2612	20030610
US 2005075333	A1	20050407	US 2004-946935	20040921

PRIORITY APPLN. INFO.:
US 2000-255241P P 20001211
US 2001-296499P P 20010606
US 2001-15532 A1 20011211
WO 2001-US47850 W 20011211
US 2002-164690 A1 20020606

OTHER SOURCE(S): MARPAT 137:337907
GI

L10 ANSWER 8 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)



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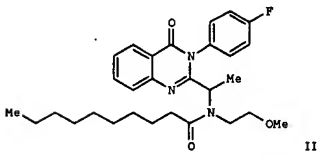


II

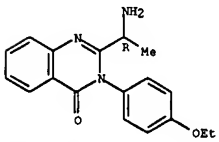
AB Title compds. I [wherein X = a bond, CO, CR5R6, CR5:, SO, SO2, or N: ; Z = a bond, N:, O, S, NR17, or CR7: ; with the proviso that X and Z are not both a bond; L = CO-alkylene or (hetero)alkylene; Q = (hetero)alkylene, CO, OCO, NR8CO, CH2CO, CH2SO, or CH2SO2; or NLQ = heterocyclyl; R1 and R2 = independently H, (hetero)alkyl, or (hetero)aryl; or CR1R2 = (hetero)cyclyl; or CNR2L = heterocyclyl; R3 = OH, alkoxy, NH2, (di)alkylamino, heteroalkyl, heterocyclyl, acylaminoamidino, guanidino, ureido, CN, heteroaryl, carbamoyl, or carboxy; R4 = (hetero)alkyl, (hetero)aryl, etc.; R5 and R6 = independently H, (hetero)alkyl, or (hetero)aryl; or CR5R6 = a ring; R7 and R8 = independently H, (hetero)alkyl, or (hetero)aryl; Y1 and Y2 = independently CR12: N:, O, S, or NR13; Y3 = N or C, wherein C shares a double bond with either Z or Y4; Y4 = NR14, CR14:, N:, NR14CR15R16; R12 = H, halo, OH, NH2, (di)alkylamino, (hetero)alkyl, or (hetero)aryl, with provisos; R13 = H, (hetero)alkyl, (hetero)aryl, etc.; R14 = (hetero)alkyl, (hetero)aryl, etc.; R15 and R16 = independently H or (hetero)alkyl; R17 = H, (hetero)alkyl, (hetero)aryl, etc.; with provisos] were prepared as chemokine receptor modulators, in particular CXCR3 antagonists. For example, anthranilic acid was acylated with propionyl chloride and the amide cyclized using acetic anhydride to give 2-ethylbenzo[d][1,3]oxazine-4-one. Treatment with 4-fluoroaniline, followed by ethylene glycol and NaOH afforded 2-ethyl-3-(4-fluorophenyl)-3H-quinazolin-4-one. Bromination and stepwise addition of 1-amino-2-methoxyethane and decanoyl chloride produced the decanoic acid (quinazolinylethyl)(methoxyethyl)amide II. Approx. one third of the 101 invention compds. tested in a CXCR3 binding assay displayed activity with IC50 values of < 1 μM. I are useful for the treatment of inflammatory and immunoregulatory disorders and diseases, such as multiple sclerosis, rheumatoid arthritis, and type I diabetes (no data).

IT 473720-85-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of N-(heteroarylalkyl)acylamides as CXCR3 antagonists for treatment of inflammatory or immune conditions)

RN 473720-85-3 CA

CN 4(3H)-Quinazolinone, 2-[(1R)-1-aminoethyl]-3-(4-ethoxyphenyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 8 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)
Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

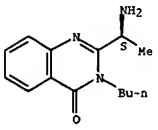
L10 ANSWER 9 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 137:63215 CA
TITLE: Traceless synthesis of 3H-quinazolin-4-ones via a combination of solid-phase and solution methodologies
AUTHOR(S): O'Mahony, Donogh J. R.; Krchnak, Viktor
CORPORATE SOURCE: SIDDCO, Inc., Tucson, AZ, 85747, USA
SOURCE: Tetrahedron Letters (2002), 43(6), 939-942
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:63215

AB A solid-phase traceless synthesis of 4-quinazolinones is described. An aldehyde functionalized resin was reductively aminated with primary amines, and the resin-bound secondary amine acylated with o-nitro-benzoic acids. The nitro group was reduced with tin(II) chloride, and the aniline acylated with acid anhydrides. Acidolytic cleavage afforded a diamide, which was cyclized in solution phase to the 4(3H)-quinazolinone removing the trace of the linker. Com. available polymer-bound 4-(4-formyl-3-methoxyphenoxy)-N-methylbutanamide was reductively aminated with 4-morpholinepropanamine, benzeneethanamine, 1-butanamine, 3-pyridinemethanamine or benzenemethanamine. The subsequent acylation of the intermediate amine was carried out using 2-nitrobenzoic acid, 5-(acetylamino)-2-nitrobenzoic acid or 4,5-dimethoxy-2-nitrobenzoic acid.

IT **439862-07-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(traceless synthesis of 3-aryl-2-alkyl-4(3H)-quinazolinone derivs. via solid-phase and solution-phase methods)

RN 439862-07-4 CA
CN 4(3H)-Quinazolinone, 2-[(1S)-1-aminoethyl]-3-butyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



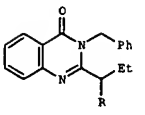
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 10 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 136:53759 CA
TITLE: Preparation of N-acylquinazolinonealkylamines as KSP kinesin inhibitors
INVENTOR(S): Finer, Jeffrey T.; Bergnes, Gustav; Feng, Bainian; Smith, Whitney W.; Chabala, John C.; Morgans, David J., Jr.
PATENT ASSIGNEE(S): Cytokinetics, Inc., USA
SOURCE: PCT Int. Appl., 179 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098278	A1	20011227	WO 2001-US13901	20010427
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6545004	B1	20030408	US 2000-699047	20001024
JP 2003048881	A2	20030221	JP 2002-156766	20001026
US 6562831	B1	20030513	US 2000-724644	20001128
US 6630479	B1	20031007	US 2000-724713	20001128
US 6831085	B1	20041214	US 2000-724941	20001128
CA 2413426	AA	20011227	CA 2001-2413426	20010427
EP 1296959	A1	20030402	EP 2001-932769	20010427
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001011898	A	20030513	BR 2001-11898	20010427
JP 2004501140	T2	20040115	JP 2002-504234	20010427
NZ 523233	A	20041029	NZ 2001-523233	20010427
ZA 2002010133	A	20030617	ZA 2002-10133	20021213
NO 2002006172	A	20030220	NO 2002-6172	20021220
US 2004023996	A1	20040205	US 2003-312323	20030815
US 2004254203	A1	20041216	US 2004-893929	20040720
PRIORITY APPLN. INFO.:			US 2000-213104P	P 20000621
			US 2000-699047	A 20001024
			US 1999-198253P	P 19991027
			JP 2001-533122	A3 20001026
			US 2000-724941	A3 20001128
			WO 2001-US13901	W 20010427

OTHER SOURCE(S): MARPAT 136:53759
GI

L10 ANSWER 10 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)



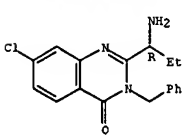
II

AB R1CR2R2'NRR4 [I; R = H, COR3, SO2R3', CH2R3''; R1 = (un)substituted 3,4-dihydro-4-oxoquinazolin-2-yl; R2,R2' = H, (oxa)alkyl, (hetero)aryl, etc.; R3 = H, alkyl, alkoxy, (hetero)aryl, etc.; R3',R4 = H, alkyl, (hetero)aryl, etc.; R3'' = alkyl, (hetero)aryl, etc.] were prepared Thus, 2-(H2N)C6H4CO2H was amidated by PrCOCl and the cyclized product cyclocondensed with PhCH2NH2 to give, after bromination, quinazolinone II (R = Br) which was converted in 2 steps to II [R = N(COC6H4F-4)CH2CH2NMe2]. Data for biol. activity of I were given.

IT **336113-55-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-acylquinazolinonealkylamines as KSP kinesin inhibitors)

RN 336113-55-4 CA
CN 4(3H)-Quinazolinone, 2-[(1R)-1-aminopropyl]-7-chloro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

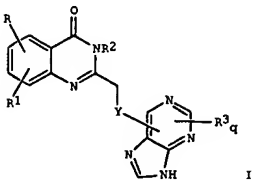


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 11 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 135:357937 CA
TITLE: Quinazolinone derivatives as inhibitors of human phosphatidylinositol 3-kinase delta
INVENTOR(S): Sadhu, Chanchal; Dick, Ken; Treiberg, Jennifer; Sowell, C. Gregory; Kesicki, Edward A.; Oliver, Amy
PATENT ASSIGNEE(S): Icos Corporation, USA
SOURCE: PCT Int. Appl., 278 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001081346	A2	20011101	WO 2001-US13315	20010424
WO 2001081346	A3	20020321		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2406278	AA	20011101	CA 2001-2406278	20010424
EP 1278748	A2	20030129	EP 2001-928855	20010424
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001010371	A	20030617	BR 2001-10371	20010424
JP 2003531209	T2	20031021	JP 2001-578436	20010424
NO 2002005104	A	20021210	NO 2002-5104	20021024
ZA 2002008698	A	20031010	ZA 2002-8698	20021028
PRIORITY APPLN. INFO.:			US 2000-199655P	P 20000425
			US 2000-238057P	P 20001005
			WO 2001-US13315	W 20010424

OTHER SOURCE(S): MARPAT 135:357937
GI



I

AB Methods of inhibiting phosphatidylinositol 3-kinase delta isoform

L10 ANSWER 11 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)

(PI3Kδ) activity, and methods of treating diseases, such as disorders of immunity and inflammation, in which PI3Kδ plays a role in leukocyte function are claimed. Preferably, the methods employ active agents that selectively inhibit PI3Kδ, while not significantly inhibiting activity of other PI3K isoforms. Compds. are provided that inhibit PI3Kδ activity, including compds. that selectively inhibit PI3Kδ activity. The compds. claimed are all quinazolin-4-one derivs., including I [Y = null, S, NH; R = H, halo, OH, OMe, Me, CF3; R1 = H, OMe, halo; RR1 together with C-6 and C-7 of quinazoline ring define a 5- or 6-membered arom. ring optionally contg. ≥ 1 O, N or S; R2 = C1-6 alkyl, Ph, halophenyl, alkylphenyl, biphenyl, PhCH2, pyridinyl, 4-methylpiperazinyl, CO2Et, morpholinyl; R3 = NH2, halo, C1-3 alkyl, S(C1-3 alkyl), OH, NH(C1-3 alkyl), N(C1-3 alkyl)2, NH(C1-3 alkylenephenyl); q = 1, 2] and pharmaceutically acceptable salts and solvates thereof. Methods of using PI3Kδ inhibitory compds. to inhibit cancer cell growth or proliferation are also provided. Accordingly, the invention provides methods of using PI3Kδ inhibitory compds. to inhibit PI3Kδ-mediated processes in vitro and in vivo. Thus, in an example, dose-dependent decrease in histamine release from basophils when stimulated with anti-IgE was 100% at 1,000 nM, with an EC50 of about 25 nM for I (Y = S, R = 5-Me, R1 = H, R2 = 2-ClC6H4, R3 = H; S connected to 6-position of purine ring; prepn. given).

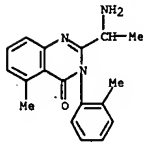
IT **371244-09-6P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and substitution reaction of, with chloropurine derivs.)

RN 371244-09-6 CA

CN 4(3H)-Quinazolinone, 2-(1-aminoethyl)-5-methyl-3-(2-methylphenyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 12 OF 19 CA COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 134:326543 CA

TITLE: Methods and compositions utilizing quinazolinones as KSP kinesin modulators

INVENTOR(S): Finer, Jeffrey T.; Bergnes, Gustave; Feng, Bainian; Smith, Whitney W.; Chabala, John C.

PATENT ASSIGNEE(S): Cytokinetics, Inc., USA

SOURCE: PCT Int. Appl., 168 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001030768	A1	20010503	WO 2000-US29585	20001026
WO 2001030768	C2	20020815		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2388646	AA	20010503	CA 2000-2388646	20001026
BR 2000015110	A	20020702	BR 2000-15110	20001026
EP 1226129	A1	20020731	EP 2000-976656	20001026
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003048881	A2	20030221	JP 2002-156766	20001026
JP 2003512461	T2	20030402	JP 2001-533122	20001026
NZ 518480	A	20040227	NZ 2000-518480	20001026
AU 774748	B2	20040708	AU 2001-14398	20001026
US 6562831	B1	20030513	US 2000-724644	20001128
US 6630479	B1	20031007	US 2000-724713	20001128
US 6831085	B1	20041214	US 2000-724941	20001128
ZA 2002002930	A	20021028	ZA 2002-2930	20020415
NO 2002001907	A	20020607	NO 2002-1907	20020423
ZA 2002010133	A	20030617	ZA 2002-10133	20021213
US 2004254203	A1	20041216	US 2004-893929	20040720

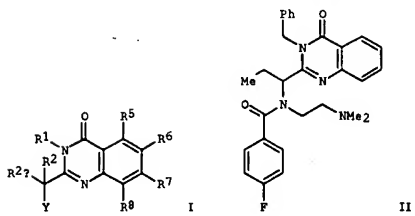
PRIORITY APPLN. INFO.:

US 1999-198253P	P	19991027
US 2000-213104P	P	20000621
US 2000-699047	A1	20001024
JP 2001-533122	A3	20001026
WO 2000-US29585	W	20001026
US 2000-724941	A3	20001128

OTHER SOURCE(S): MARPAT 134:326543

GI

L10 ANSWER 12 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)



I

II

AB Quinazolinones (I) [wherein R1 = H, alkyl, (hetero)aryl, or (un)substituted alkyl(hetero)aryl; R2 and R2a = independently H or (un)substituted (oxa)alkyl, (hetero)aryl, or alkyl(hetero)aryl; Y = NR4COR3, NR4SO2R3a, NR4CH2R3b, or NHR4; R3 = H, oxaalkyl, or (un)substituted alkyl, (hetero)aryl, alkyl(hetero)aryl, oxaalkylaryl, ether, or amino; R3a = H or (un)substituted alkyl, (hetero)aryl, alkyl(hetero)aryl, or amino; R3b = (un)substituted alkyl, (hetero)aryl, or alkyl(hetero)aryl; R4 = H or (un)substituted alkyl, (hetero)aryl, alkyl(hetero)aryl, or alkylene; R5-R8 = independently H, (fluoro)alkyl, alkoxy, halo, NO2, dialkylamino, alkylsulfonyl, alkylsulfonamido(alkyl or aryl), alkylthio, carboxyalkyl, carboxamido, aminocarbonyl, or (hetero)aryl] were prepared by conventional and solid phase combinatorial synthetic methods as KSP kinesin inhibitors for treatment of cellular proliferative diseases. For example, II was synthesized in a 6-step sequence involving (1) amidation of anthranilic acid with butyryl chloride (65%), (2) cyclization to give 2-propyl-3,1-[4H]benzoxazin-4-one (62%), (3) treatment with PhCH2NH2 to give 2-propyl-3-benzylquinazolin-4-one (67%), bromination (92%), addition of N,N-dimethylethylenediamine (55%), and (6) amidation with p-fluorobenzoyl chloride (65%). I are useful for treating cancer, hyperplasia, restenosis, cardiac hypertrophy, immune disorders, and inflammation (no data). Methods of screening for compds. that will bind to a KSP kinesin or are modulators of KSP kinesin activity are also disclosed.

IT **336113-55-4P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

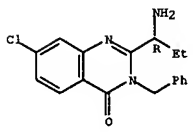
(preparation of quinazolinone KSP kinesin modulators via conventional and solid phase combinatorial synthetic methods)

RN 336113-55-4 CA

CN 4(3H)-Quinazolinone, 2-[(1R)-1-aminopropyl]-7-chloro-3-(phenylmethyl)- (9CI) (CA INDEX NAME)

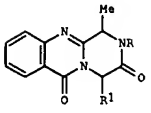
Absolute stereochemistry.

L10 ANSWER 12 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 13 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 130:38348 CA
TITLE: Nitrogen bridgehead compounds. Part 90. An efficient versatile synthesis of 1-methyl-2-substituted 1,2,3,4-tetrahydro-6H-pyrazino[2,1-b]quinazoline-3,6-diones
AUTHOR(S): Kokosi, Jozsef; Almasi, Janos; Podanyi, Benjamin; Feher, Miklos; Bocskei, Zsolt; Simon, Kalman; Hermecz, Istvan
CORPORATE SOURCE: Institute for Pharmaceutical Chemistry Semmelweis University of Medicine, Budapest, 1092, Hung.
SOURCE: Heterocycles (1998), 48(9), 1851-1866
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:38348
GI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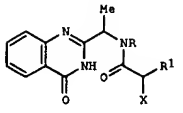
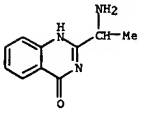

II

AB A versatile synthesis of 2-substituted 1-methyl- and 1,4-dimethyl-1,2,3,4-tetrahydro-6H-pyrazino[2,1-b]quinazoline-3,6-diones I (R = H, Et, Ph, etc., R1 = H, Me) is presented, starting from 2-(1-bromoethyl)quinazolin-4(3H)-one. The key step of the reaction sequence is the diastereoselective cyclization of 2-{[1-(N-2-haloacyl)-N-substituted amino]ethyl}quinazolin-4(3H)-ones II (R1 = H, X = Cl; R1 = Me, X = Br). Usually 1,4-di-Me derivs. are obtained as pure racemic cis-compds. (2-alkyl and 2-benzyl derivs.), or a mixture of diastereomers, containing the 4-Me group in quasi-axial position.

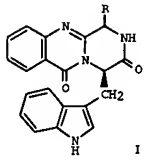
IT 172420-42-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of methylpyrazinoquinazolinediones)

RN 172420-42-7 CA
CN 4(1H)-Quinazolinone, 2-(1-aminoethyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 13 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 14 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 128:257597 CA
TITLE: Total Synthesis of the Quinazoline Alkaloids (-)-Fumiquinazoline G and (-)-Fiscalin B
AUTHOR(S): Wang, Haishan; Ganesan, A.
CORPORATE SOURCE: Institute of Molecular and Cell Biology, National University of Singapore, Singapore, 117609, Singapore
SOURCE: Journal of Organic Chemistry (1998), 63(8), 2432-2433
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:257597
GI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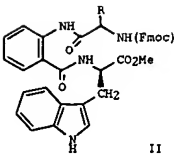
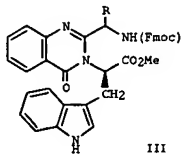

II


III

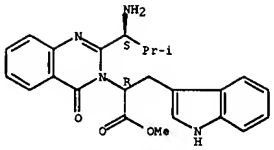
AB (-)-Fumiquinazoline G (I; R = β-Me) and (-)-fiscalin B (I; R = α-CHMe2) were synthesized in four and five steps resp. from D-tryptophan Me ester. The key transformation involved dehydrative cyclization of linear tripeptides II (Fmoc = 9-fluorenylmethoxycarbonyl, R = β-Me, α-CHMe2, resp.) to quinazolin-4-ones III. The methodol. is also applicable to the synthesis of quinazolinones with sterically bulky 2,3-substitution.

IT 205042-99-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of the quinazoline alkaloids fumiquinazoline G and fiscalin B from D-tryptophan Me ester)

RN 205042-99-5 CA
CN 3(4H)-Quinazolineacetic acid, 2-(1-amino-2-methylpropyl)-α-(1H-indol-3-ylmethyl)-4-oxo-, methyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

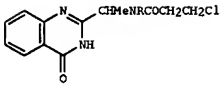
Absolute stereochemistry.

L10 ANSWER 14 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)

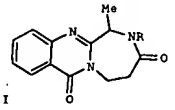


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 15 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 125:328537 CA
TITLE: Synthesis and cyclization of new quinazolone derivatives to [1,4]oxazepino- and [1,4]diazepino[3,4-b]quinazolones
AUTHOR(S): Szabo, Monika; Orfi, Laszlo; Kokosi, Jozsef; Hermecz, Istvan; Kovacs, Attila
CORPORATE SOURCE: Semmelweis Orvostudomanyi Egyetem, Gyogyszereszi Kemiai Intezet, Budapest, 1092, Hung.
SOURCE: Magyar Kemiai Folyoirat (1996), 102(8), 343-355
CODEN: MGKFA3; ISSN: 0025-0155
PUBLISHER: Magyar Kemikusok Egyesulete
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
GI

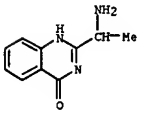


I

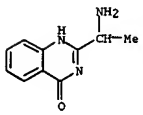


II

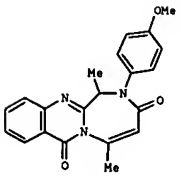
AB Original routes have been developed for the synthesis of new heterocondensed quinazolones: [1,4]oxazepino[3,4-b]quinazolone and [1,4]diazepino[3,4-b]quinazolones. E.g., cyclization of quinazolone I (R = 4-MeOC6H4) gave [1,4]diazepino[3,4-b]quinazolone II.
IT 172420-42-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of quinazolones, [1,4]oxazepino-, and [1,4]diazepino[3,4-b]quinazolones)
RN 172420-42-7 CA
CN 4(1H)-Quinazolinone, 2-(1-aminoethyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 16 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)



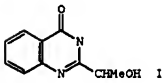
L10 ANSWER 16 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 124:86929 CA
TITLE: Synthesis of potential CCK antagonist quinazolone derivatives
AUTHOR(S): Szabo, Monika; Kokosi, Jozsef; Orfi, Laszlo
CORPORATE SOURCE: Gyogyszereszi Kemiai Intezet, Semmelweis Orvostudomanyi Egyetem, Budapest, Hung.
SOURCE: Acta Pharmaceutica Hungarica (1995), 65(4), 133-8
CODEN: APHGAO; ISSN: 0001-6659
PUBLISHER: Ifjusagi Lap- es Konyvkiado Vallalat
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
GI



I

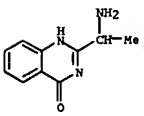
AB An original route has been found for the synthesis of [1,4]diazepinoquinazolones (e.g., I), a new ring system of heterocondensed quinazolones. These anthranilic acid-alanine-β-alanine cyclopeptide derivs. constitute a structural moiety of asperlicin, the first natural cholecystokinin antagonist alkaloid. These compds. are therefore potential CCK antagonists. The new compds. were prepared via condensation of 2-(aminoalkyl)quinazolones, obtained from 2-alkylquinazolones by side-chain substitution, with 1,3-bifunctional reagents. We studied the cyclization process under basic, acidic and phase-transfer catalyzed conditions. The structures of the synthesized compds. were characterized by IR, UR and NMR spectroscopy.
IT 172420-42-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of [1,4]diazepinoquinazolones as potential CCK antagonists)
RN 172420-42-7 CA
CN 4(1H)-Quinazolinone, 2-(1-aminoethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 17 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 113:171734 CA
TITLE: Synthesis of chrysogine, a metabolite of Penicillium chrysogenum and some related 2-substituted 4-(3H)-quinazolinones
AUTHOR(S): Bergman, Jan; Brynolf, Anna
CORPORATE SOURCE: Dep. Org. Chem., R. Inst. Technol., Stockholm, S-100 44, Swed.
SOURCE: Tetrahedron (1990), 46(4), 1295-310
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:171734
GI



I

AB Both enantiomers of chrysogine (I) were prepared from 2-H2NC6H4CONH2 (II). Thus reaction of II and (-)-AcOCHMeCOCl gave (-)-2-AcOCHMeCONHC6H4CONH2 which upon saponification and cyclization induced by aqueous Na2CO3 at room temperature gave (S)-(-)-I. The enantiomeric purity of (S)-(-)-I was determined by NMR. Inversion of (-)-(S)-I using the Mitsunobu reaction, gave (+)-(R)-I. Reduction of 2-acetyl-4(3H)-quinazolinone with bakers' yeast gave (S)-(-)-I. The cyclization method could be extended to a number of 2-(α-hydroxy)alkyl-4-(3H)-quinazolinones.
IT 172420-42-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and trifluoroacetylation of)
RN 172420-42-7 CA
CN 4(1H)-Quinazolinone, 2-(1-aminoethyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 18 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 110:135739 CA
TITLE: Preparation of 4-amino-3-hydroxy-5-cyclohexylpentanoyl-containing peptides as renin inhibitors
INVENTOR(S): Gante, Joachim; Raddatz, Peter; Sombroek, Johannes; Schmitges, Claus J.; Minck, Klaus Otto
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 17 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3721855	A1	19880922	DE 1987-3721855	19870702
EP 286813	A2	19881019	EP 1988-102971	19880229
EP 286813	A3	19901212		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
AU 8812617	A1	19880915	AU 1988-12617	19880301
AU 614951	B2	19910919		
JP 63258451	A2	19881025	JP 1988-56504	19880311
ZA 8801782	A	19881026	ZA 1988-1782	19880311
HU 49147	A2	19890828	HU 1988-1191	19880311
HU 204848	B	19920228		
PRIORITY APPLN. INFO.:			DE 1987-3707879	A1 19870312
			DE 1987-3721855	A 19870702

OTHER SOURCE(S): MARPAT 110:135739

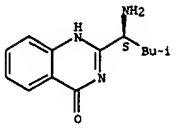
AB X-Z-NR2-CHR3-CR4-(CHR5)n-CO-E-NR6-D [I; X = H, R1O(CH2)mCO, R1SO2, etc.; Z = 0-4 amino acid residues chosen from Abu, Ada, Ala, β-Ala, Arg, Asn, Asp, Bia, Cal, Dab, Gln, Glu, Gly, His, N(i.m.)-alkyl-His, Ile, Leu, tert-Leu, Lys, Met, α-Nal, β-Nal, Nbg, Nle, Orn, Phe, Pro, Ser, Thr, Tic, Trp, Tyr, Val; E = 0-2 amino acid residues chosen from Abu, Ala, Cal, His, Ile, Leu, Met, Nle, Phe, Trp, Tyr, Val; D = CH2CH(OH)CH2OH, (CH2)zSO2R7, phenylalkyl, furylalkyl, thienylalkyl, pyridylalkyl, etc.; R1, R3 = H, aryl, arylalkyl, heterocyclyl, heterocyclylalkyl, (substituted) C3-7 cycloalkyl, etc.; R2, R5, R6 = H, alkyl; R4 = :O, (H,OH), (H,NH2); R7 = OH, alkoxy, amino; m = 0-5; n = 1, 2; z = 2-6; Bia = 3-(2-benzimidazolyl)alanyl; Cal = 3-cyclohexylalanyl; Dab = 2,4-diaminobutyryl; α-Nal = α-naphthylalanyl; β-Nal = β-naphthylalanyl, Nbg = (2-norbornyl)glycyl; Tic = tetrahydroisoquinolinyl-1-carbonyl], useful as renin inhibitors (no data), were prepared 2-[1S-(3S-Hydroxy-4S-(N-tert-butoxycarbonylphenylalanylhistidylamino)-5-cyclohexylpentanoylamino)-3-methylbutyl]-3H-quinazolin-4-one was prepared by the solution phase method.

IT **119422-37-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as renin inhibitor intermediate)

RN 119422-37-6 CA
CN 4(1H)-Quinazolinone, 2-(1-amino-3-methylbutyl)-, dihydrochloride, (S)- (9CI) (CA INDEX NAME)

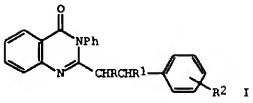
Absolute stereochemistry.

L10 ANSWER 18 OF 19 CA COPYRIGHT 2005 ACS on STN (Continued)



●2 HCl

L10 ANSWER 19 OF 19 CA COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 94:175028 CA
TITLE: Reactions of 2,3-disubstituted 4(3H)-quinazolinones and related compounds
AUTHOR(S): Badr, M. Z. A.; El-Naggar, G. M.; El-Sherief, H. A. H.
CORPORATE SOURCE: Fac. Sci., Assiut Univ., Assiut, Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1980), 19B(10), 925-6
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 94:175028
GI

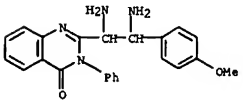


I

AB The arylidenequinazolines I (RR1 = bond, R2 = p-MeO, H, m-NO2, p-NO2) were brominated with Br2 to give I (R = R1 = Br). I (R = R1 = Br, R2 = p-MeO) underwent substitution reactions to give I (R = Br, R1 = AcO, MeO, EtO; R = R1 = H2N, piperidino, morpholino, PhO, PhS; R2 = p-MeO). I (RR1 = bond, R2 = p-MeO) was also obtained as an elimination product.

IT **77143-54-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 77143-54-5 CA
CN 4(3H)-Quinazolinone, 2-[1,2-diamino-2-(4-methoxyphenyl)ethyl]-3-phenyl- (9CI) (CA INDEX NAME)



10/773,602

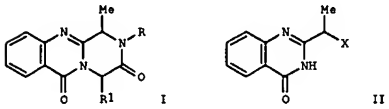
=> file casreact

=> s l7 full

L12 6 SEA SSS FUL L7 (17 REACTIONS)

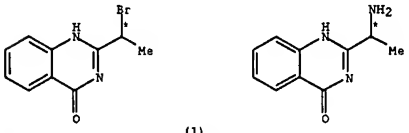
=> d ibib abs rx 1-6

L12 ANSWER 1 OF 6 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 141:23488 CASREACT
TITLE: A preparation of pyrazino[2,1-b]quinazolone derivatives useful as multidrug resistance modulators
AUTHOR(S): Kokosi, Jozsef; Almasi, Janos; Podanyi, Benjamin; Hermecz, Istvan
CORPORATE SOURCE: Gyogyszereszi Kemiai Intezet, Semmelweis Egyetem, Budapest, Russia
SOURCE: Acta Pharmaceutica Hungarica (2003), 73(1), 29-39
CODEN: APHGAO; ISSN: 0001-6659
PUBLISHER: Magyar Gyogyszereszeti Tarsasag
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
GI



AB An exploration for new MDR-modulators utilizing pyrazino[2,1-b]quinazolones as scaffolds disclosed after systematic synthetic investigation highly hydrophobic N-substituted derivs. as readily accessible active tricyclic compds. (no biol. data). A versatile synthesis of 2-substituted-1,2,3,4-tetrahydro-6H-pyrazino[2,1-b]quinazoline-3,6-diones is presented starting from 2,3-substituted quinazolones. The new compds. have been characterized by elemental analyses, NMR, and in some cases by 13C ruler, and X-ray investigations. For instance, pyrazino[2,1-b]quinazoline derivative I was prepared via amination of quinazoline II (X = Br) by RNH2, N-acetylation of the obtained amine II (X = NHR) by YCH(R1)C(O)Y (R1 is H or Me; Y is Cl or Br), and subsequent heterocyclization of the obtained amide II [X = N(R)C(O)C(Y)R1].

RX(1) OF 147 A ===> B...

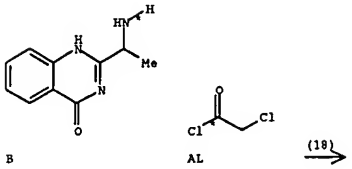


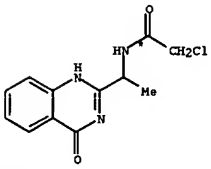
YIELD 72%

L12 ANSWER 1 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

RX(1) RCT A 144189-81-1
RGT C 7664-41-7 NH3
PRO B 172420-42-7
SOL 64-17-5 EtOH

RX(18) OF 147 ...B + AL ===> AM...





YIELD 60%

RX(18) RCT B 172420-42-7

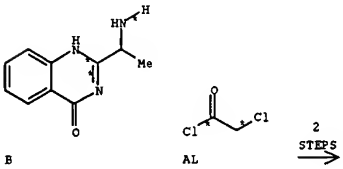
STAGE(1)
SOL 67-66-3 CHCl3

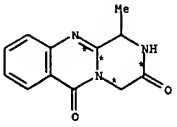
STAGE(2)
RCT AL 79-04-9

STAGE(3)
RGT AN 110-86-1 Pyridine
PRO AM 216596-07-5

L12 ANSWER 1 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

RX(92) OF 147 COMPOSED OF RX(18), RX(41)
RX(92) B + AL ===> BO





YIELD 88%

RX(18) RCT B 172420-42-7

STAGE(1)
SOL 67-66-3 CHCl3

STAGE(2)
RCT AL 79-04-9

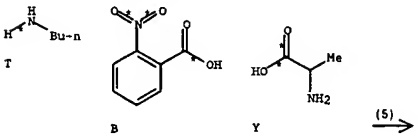
STAGE(3)
RGT AN 110-86-1 Pyridine
PRO AM 216596-07-5

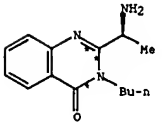
RX(41) RCT AM 216596-07-5
RGT S 141-52-6 NaOEt
PRO BO 204770-75-2
SOL 64-17-5 EtOH
NTE key step

L12 ANSWER 2 OF 6 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 137:63215 CASREACT
TITLE: Traceless synthesis of 3H-quinazolin-4-ones via a combination of solid-phase and solution methodologies
AUTHOR(S): O'Mahony, Donogh J. R.; Krchnak, Viktor
CORPORATE SOURCE: SIDDCO, Inc., Tucson, AZ, 85747, USA
SOURCE: Tetrahedron Letters (2002), 43(6), 939-942
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A solid-phase traceless synthesis of 4-quinazolinones is described. An aldehyde functionalized resin was reductively aminated with primary amines, and the resin-bound secondary amine acylated with o-nitro-benzoic acids. The nitro group was reduced with tin(II) chloride, and the aniline acylated with acid anhydrides. Acidolytic cleavage afforded a diamide, which was cyclized in solution phase to the 4(3H)-quinazolinone removing the trace of the linker. Com. available polymer-bound 4-(4-formyl-3-methoxyphenoxy)-N-methylbutanamide was reductively aminated with 4-morpholinepropanamine, benzeneethanamine, 1-butanamine, 3-pyridinemethanamine or benzenemethanamine. The subsequent acylation of the intermediate amine was carried out using 2-nitrobenzoic acid, 5-(acetylamino)-2-nitrobenzoic acid or 4,5-dimethoxy-2-nitrobenzoic acid.

RX(5) OF 7 T + B + Y ===> Z





YIELD 19%

RX(5) RCT T 109-73-9, B 552-16-9

STAGE(1)
RGT E 693-13-0 i-PrN:C:NPr-i, F 2592-95-2 1-Benzotriazolol
SOL 68-12-2 DMF

L12 ANSWER 2 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

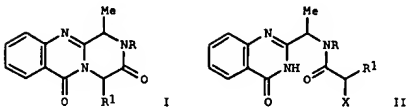
STAGE(2)
RGT G 7772-99-8 SnCl2, H 7087-68-5 EtN(Pr-i)2
SOL 872-50-4 NMEP

STAGE(3)
RCT Y 56-41-7
RGT E 693-13-0 i-PrN:C:NPr-i, I 110-86-1 Pyridine
SOL 123-91-1 Dioxane

STAGE(4)
RGT J 7664-39-3 HF

STAGE(5)
RGT K 75-77-4 Me3SiCl, L 598-56-1 EtNMe2
SOL 75-05-8 MeCN
PRO Z 439862-07-4
NTE solid-supported reaction
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

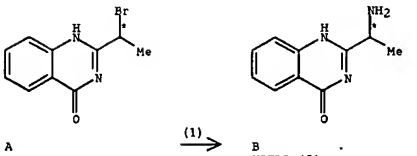
L12 ANSWER 3 OF 6 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 130:38348 CASREACT
TITLE: Nitrogen bridgehead compounds. Part 90. An efficient versatile synthesis of 1-methyl-2-substituted 1,2,3,4-tetrahydro-6H-pyrazino[2,1-b]quinazoline-3,6-diones
AUTHOR(S): Kokosi, Jozsef; Almasi, Janos; Podanyi, Benjamin; Feher, Miklos; Bocskei, Zsolt; Simon, Kalman; Hermecz, Istvan
CORPORATE SOURCE: Institute for Pharmaceutical Chemistry Semmelweis University of Medicine, Budapest, 1092, Hung.
SOURCE: Heterocycles (1998), 48(9), 1851-1866
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB A versatile synthesis of 2-substituted 1-methyl- and 1,4-dimethyl-1,2,3,4-tetrahydro-6H-pyrazino[2,1-b]quinazoline-3,6-diones I (R = H, Et, Ph, etc., R1 = H, Me) is presented, starting from 2-(1-bromoethyl)quinazolin-4(3H)-one. The key step of the reaction sequence is the diastereoselective cyclization of 2-{[1-(N-2-haloacyl)-N-substituted amino]ethyl}quinazolin-4(3H)-ones II (R1 = H, X = Cl; R1 = Me, X = Br). Usually 1,4-di-Me derivs. are obtained as pure racemic cis-compds. (2-alkyl and 2-benzyl derivs.), or a mixture of diastereomers, containing the 4-Me group in quasi-axial position.

RX(1) OF 100 A ===> B...

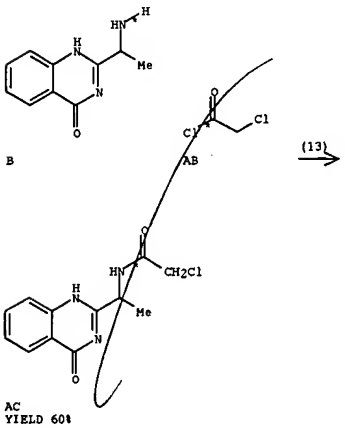
L12 ANSWER 3 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



A
B
YIELD 45%

RX(1) RCT A 144189-81-1
RGT C 7664-41-7 NH3
PRO B 172420-42-7
SOL 64-17-5 EtOH
NTE Et, Pr, and Bu analogs similarly prepd. in 75-77% yields

RX(13) OF 100 ...B + AB ===> AC...

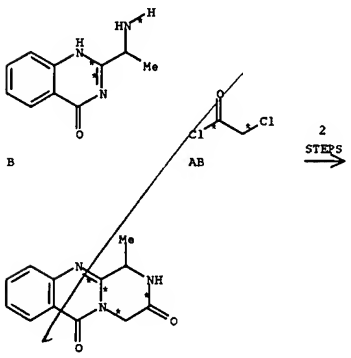


B
AB
AC
YIELD 60%

RX(13) RCT B 172420-42-7, AB 79-04-9
RGT AD 110-86-1 Pyridine

L12 ANSWER 3 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)
PRO AC 216596-07-5
SOL 67-66-3 CHCl3

RX(60) OF 100 COMPOSED OF RX(13), RX(27)
RX(60) B + AB ===> AV

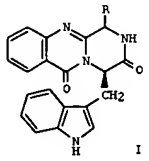


B
AB
AV
YIELD 88%

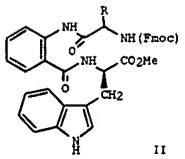
RX(13) RCT B 172420-42-7, AB 79-04-9
RGT AD 110-86-1 Pyridine
PRO AC 216596-07-5
SOL 67-66-3 CHCl3

RX(27) RCT AC 216596-07-5
RGT AW 141-52-6 NaOEt
PRO AV 204770-75-2
SOL 64-17-5 EtOH
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

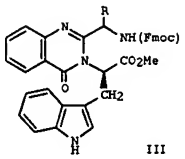
L12 ANSWER 4 OF 6 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 128:257597 CASREACT
TITLE: Total Synthesis of the Quinazoline Alkaloids (-)-Fumiquinazoline G and (-)-Fiscalin B
AUTHOR(S): Wang, Haishan; Ganesan, A.
CORPORATE SOURCE: Institute of Molecular and Cell Biology, National University of Singapore, Singapore, 117609, Singapore
SOURCE: Journal of Organic Chemistry (1998), 63(8), 2432-2433
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

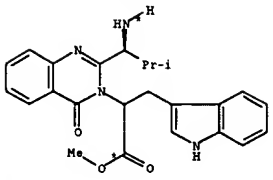


III

AB (-)-Fumiquinazoline G (I; R = β-Me) and (-)-fiscalin B (I; R = α-CHMe2) were synthesized in four and five steps resp. from D-tryptophan Me ester. The key transformation involved dehydrative cyclization of linear tripeptides II (Fmoc = 9-fluorenylmethoxycarbonyl, R = β-Me, α-CHMe2, resp.) to quinazolin-4-ones III. The methodol. is also applicable to the synthesis of quinazolinones with sterically bulky 2,3-substitution.

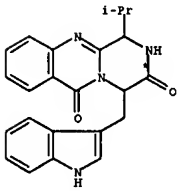
RX(2) OF 20 E ===> F

L12 ANSWER 4 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



E

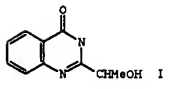
(2)



F
YIELD 72%

RX(2) RCT E 205042-99-5
STAGE(1)
RGT C 110-89-4 Piperidine
SOL 75-09-2 CH2Cl2
STAGE(2)
RGT G 1122-58-3 4-DMAP
SOL 75-05-8 MeCN
PRO F 149008-35-5
NTE 2nd stage reflux
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

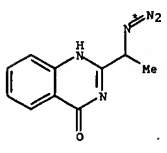
L12 ANSWER 5 OF 6 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 113:171734 CASREACT
TITLE: Synthesis of chrysogine, a metabolite of Penicillium chrysogenum and some related 2-substituted 4-(3H)-quinazolinones
AUTHOR(S): Bergman, Jan; Brynolf, Anna
CORPORATE SOURCE: Dep. Org. Chem., R. Inst. Technol., Stockholm, S-100 44, Swed.
SOURCE: Tetrahedron (1990), 46(4), 1295-310
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

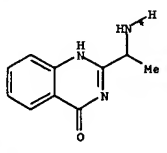
AB Both enantiomers of chrysogine (I) were prepared from 2-H2NC6H4CONH2 (II). Thus reaction of II and (-)-AcOCHMeCOCl gave (-)-2-AcOCHMeCONHC6H4CONH2 which upon saponification and cyclization induced by aqueous Na2CO3 at room temperature gave (S)-(-)-I. The enantiomeric purity of (S)-(-)-I was determined by NMR. Inversion of (-)-(S)-I using the Mitsunobu reaction, gave (+)-(R)-I. Reduction of 2-acetyl-4(3H)-quinazolinone with bakers' yeast gave (S)-(-)-I. The cyclization method could be extended to a number of 2-(α-hydroxy)alkyl-4-(3H)-quinazolinones.

RX(27) OF 82 ...AQ ===> AS...



AQ

(27)

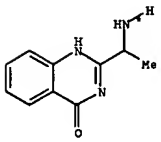


AS
YIELD 98%

RX(27) RCT AQ 129768-59-8
PRO AS 172420-42-7

RX(30) OF 82 ...AS + AW ===> AV

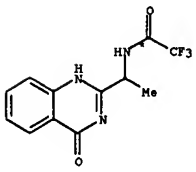
L12 ANSWER 5 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



AS

AW

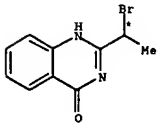
(30)



AV

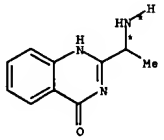
RX(30) RCT AS 172420-42-7, AW 76-05-1
PRO AV 129768-62-3
CAT 144-55-8 NaHCO3

RX(52) OF 82 COMPOSED OF RX(26), RX(27)
RX(52) AO ===> AS



AO

2 STEPS



AS
YIELD 98%

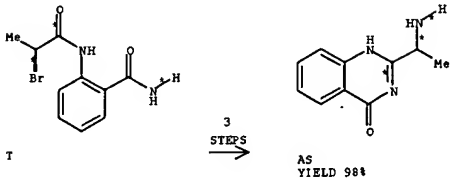
RX(26) RCT AO 144189-81-1

L12 ANSWER 5 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

RGT AR 26628-22-8 NaN3
PRO AQ 129768-59-8

RX(27) RCT AQ 129768-59-8
PRO AS 172420-42-7

RX(72) OF 82 COMPOSED OF RX(24), RX(26), RX(27)
RX(72) T ===> AS



T

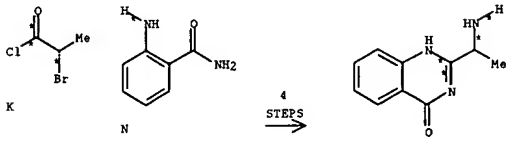
AS
YIELD 98%

RX(24) RCT T 129831-32-9
PRO AO 144189-81-1
CAT 104-15-4 TsOH

RX(26) RCT AO 144189-81-1
RGT AR 26628-22-8 NaN3
PRO AQ 129768-59-8

RX(27) RCT AQ 129768-59-8
PRO AS 172420-42-7

RX(73) OF 82 COMPOSED OF RX(11), RX(24), RX(26), RX(27)
RX(73) K + N ===> AS



K

N

AS
YIELD 98%

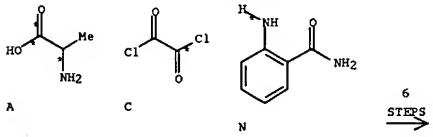
L12 ANSWER 5 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

CAT 104-15-4 TsOH

RX(26) RCT AO 144189-81-1
RGT AR 26628-22-8 NaN3
PRO AQ 129768-59-8

RX(27) RCT AQ 129768-59-8
PRO AS 172420-42-7

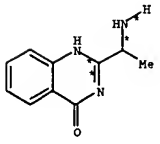
RX(79) OF 82 COMPOSED OF RX(3), RX(6), RX(11), RX(24), RX(26), RX(27)
RX(79) A + C + N ===> AS



A

C

N



AS
YIELD 98%

RX(3) RCT A 56-41-7
PRO E 32644-15-8

RX(6) RCT E 32644-15-8, C 79-37-8
PRO K 22592-73-0

RX(11) RCT K 22592-73-0, N 88-68-6
PRO T 129831-32-9

RX(24) RCT T 129831-32-9
PRO AO 144189-81-1
CAT 104-15-4 TsOH

RX(26) RCT AO 144189-81-1
RGT AR 26628-22-8 NaN3
PRO AQ 129768-59-8

RX(27) RCT AQ 129768-59-8

L12 ANSWER 5 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

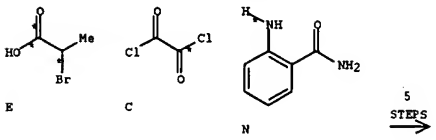
RX(11) RCT K 22592-73-0, N 88-68-6
PRO T 129831-32-9

RX(24) RCT T 129831-32-9
PRO AO 144189-81-1
CAT 104-15-4 TsOH

RX(26) RCT AO 144189-81-1
RGT AR 26628-22-8 NaN3
PRO AQ 129768-59-8

RX(27) RCT AQ 129768-59-8
PRO AS 172420-42-7

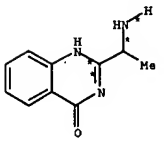
RX(78) OF 82 COMPOSED OF RX(6), RX(11), RX(24), RX(26), RX(27)
RX(78) E + C + N ===> AS



E

C

N



AS
YIELD 98%

RX(6) RCT E 32644-15-8, C 79-37-8
PRO K 22592-73-0

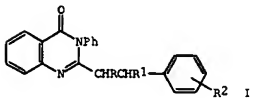
RX(11) RCT K 22592-73-0, N 88-68-6
PRO T 129831-32-9

RX(24) RCT T 129831-32-9
PRO AO 144189-81-1

L12 ANSWER 5 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

PRO AS 172420-42-7

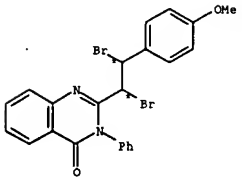
L12 ANSWER 6 OF 6 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 94:175028 CASREACT
TITLE: Reactions of 2,3-disubstituted 4(3H)-quinazolinones and related compounds
AUTHOR(S): Badr, M. Z. A.; El-Naggar, G. M.; El-Sherief, H. A. H.
CORPORATE SOURCE: Fac. Sci., Assiut Univ., Assiut, Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1980), 19B(10), 925-6
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The arylidenequinazolines I (RR1 = bond, R2 = p-MeO, H, m-NO2, p-NO2) were brominated with Br2 to give I (R = R1 = Br). I (R = R1 = Br, R2 = p-MeO) underwent substitution reactions to give I (R = Br, R1 = AcO, MeO, EtO; R = R1 = H2N, piperidino, morpholino, PhO, PhS; R2 = p-MeO). I (RR1 = bond, R2 = p-MeO) was also obtained as an elimination product.

RX(12) OF 25 ...F ===> Q



F

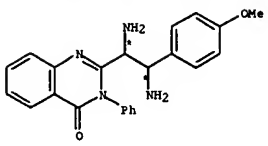
(12)

L12 ANSWER 6 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)

RX(7) RCT G 77143-59-0
RGT C 7726-95-6 Br2
PRO F 77143-47-6

RX(12) RCT F 77143-47-6
RGT R 7664-41-7 NH3
PRO Q **77143-54-5**

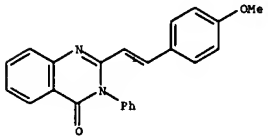
L12 ANSWER 6 OF 6 CASREACT COPYRIGHT 2005 ACS on STN (Continued)



Q

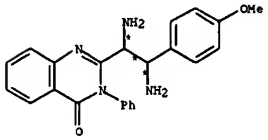
RX(12) RCT F 77143-47-6
RGT R 7664-41-7 NH3
PRO Q **77143-54-5**

RX(21) OF 25 COMPOSED OF RX(7), RX(12)
RX(21) G ===> Q



G

2 STEPS



Q

10/773,602

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FILE 'REGISTRY' ENTERED AT 09:25:50 ON 19 APR 2005
L1 STRUCTURE UPLOADED
L2 0 S L1 SAM
L3 1 S L1 FULL

FILE 'CA' ENTERED AT 09:26:26 ON 19 APR 2005
L4 1 S L3

FILE 'CASREACT' ENTERED AT 09:26:37 ON 19 APR 2005
L5 0 S L1
L6 0 S L1 FULL
L7 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 09:27:51 ON 19 APR 2005
L8 1 S L7
L9 23 S L7 FULL

FILE 'CA' ENTERED AT 09:28:11 ON 19 APR 2005
L10 19 S L9

FILE 'CASREACT' ENTERED AT 09:28:31 ON 19 APR 2005
L11 1 S L7 SAM
L12 6 S L7 FULL